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Validation of ENVISAT/SCIAMACHY columnar CO by FTIR profile retrievals at the Ground-Truthing Station Zugspitze

R. Sussmann[1] **and M. Buchwitz**[2]

[1]IMK-IFU, Forschungszentrum Karlsruhe, Garmisch-Partenkirchen, Germany
[2]Institute of Environmental Physics (iup), University of Bremen FB1, Bremen, Germany

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Correspondence to: R. Sussmann (ralf.sussmann@imk.fzk.de)

Abstract

Carbon monoxide vertical profile retrievals from ground-based solar FTIR measurements at the Permanent Ground-Truthing Station Zugspitze (47.42° N, 10.98° E, 2964 m a.s.l.), Germany are used to validate columnar CO retrieved from ENVISAT/SCIAMACHY spectra (WFM-DOAS version 0.4). The WFM-DOAS retrievals of CO include an empirical column scaling factor of 0.5. Therefore, not absolute column levels are validated, but the proper response of the SCIAMACHY retrievals to the atmospheric inter-annual variability is quantitatively assessed in comparison to the Zugspitze FTIR results. Although CO WFM-DOAS data for only 33 days are available up to now (data covering January–October 2003), it is possible to retrieve information on the CO annual cycle (≈10% amplitude) in a statistically significant fit out of the scatter of the SCIAMACHY WFM-DOAS data. To obtain this, all pixels within a minimum radius of 2000 km around Zugspitze had to be averaged for each day.

1. Introduction

Carbon monoxide (CO) is one of the key reactive species in troposheric chemistry (IPCC, 2001). The investigation of its global distribution has again gained high-priority interest only recently, due to the detection of its hitherto unrecorded and probably unprecedented column enhancements by up to >50% for several months in the 1998 northern hemisphere (Yurganov et al., 2004), and similar follow-on anomalies found in 2002 and 2003. This has been assessed quantitatively by a group of ground-based solar FTIR (Fourier Transform Infrared) spectrometry sites operated within the NDSC (Network for the Detection of Stratospheric Change) complemented by in-situ surface-sampling sites of the GAW (Global Atmosphere Watch) network. These ground networks are performing with high precisions which are better than 2–3% (FTIR) and better than 5% (in situ), respectively.

Currently, there is only one fully validated space-borne remote sounder that can add information on the global distribution of CO to the highly precise ground-based networks, i.e., the MOPITT (Measurements Of Pollution In The Troposphere) instrument mounted on the EOS-Terra platform (Deeter et al., 2003). Meanwhile, another satellite instrument has achieved the potential to retrieve global information on CO, i.e., the Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY (SCIAMACHY), which is a UV/visible/NIR spectrometer onboard ENVISAT launched in 2002 (Bovensmann et al., 1999). In this paper we focus on the validation of the SCIAMACHY scientific total column product for the species CO (WFM-DOAS, ver. 0.4), retrieved at the University of Bremen (Buchwitz and Burrows, 2004; Buchwitz et al., 2004). A set of CO columns for 33 different days out of the time span January–October 2003 has been released to the public in early 2004 via the internet (http://www.iup.physik.uni-bremen.de/sciamachy/NIR_NADIR_WFM_DOAS/). This scientific product plays a key role for the users community, since there has been no operational SCIAMACHY product for CO released by ESA yet.

A first validation study for the WFM-DOAS (WFMD) CO retrievals had been performed by comparing with data of the MOPITT satellite instrument. A highly consistent behavior relative to MOPITT had been found in the capability to detect highly elevated CO columns, e.g., a plume from biomass burning (Buchwitz et al., 2004). During this study, empirical scaling factors of 0.5 have been established for the WFMD CO column retrievals which resulted from an adaptation to the MOPITT CO data, and will remain unchanged for the next algorithm version updates (Buchwitz et al., 2004). Therefore, it is no issue for current validation studies to assess the overall absolute accuracy of the WFMD CO columns. The issue of validation is therefore now to asses the ability of the WFM-DOAS retrievals to monitor the real atmospheric variability of CO columns in a realistic manner.

In this paper we want to promote the validation of CO by comparing the WFMD retrievals to the ground-based correlative solar FTIR data of the clean air site Zugspitze. The question to be addressed in this study, is whether the WFMD retrievals can reflect the natural variability of CO above the clean air site Zugspitze, which is dominated by the annual cycle for this species.

2. The correlative ground data set from Zugspitze solar FTIR

For details of the SCIAMACHY WFMD CO retrievals in the near-infrared spectral domain, the reader is referred to Buchwitz and Burrows (2004) and Buchwitz et al. (2004). Validation is performed using the correlative ground-based data that are being recorded by the NDSC Primary Status solar FTIR instrument at the Zugspitze (47.42° N, 10.98° E, 2964 m a.s.l.) continuously. The Zugspitze FTIR-instrument and retrieval-set up has been described in detail elsewhere (Sussmann, 1997, 1999). Briefly, a high-resolution Bruker IFS 120 HR Fourier Transform Spectrometer is operated with an actively controlled solar tracker, and liquid-nitrogen cooled MCT and InSb detectors. For the CO retrievals, interferograms with a maximum optical path difference (OPD) of 250 cm are recorded. Typically, 6 individual interferograms are averaged to obtain one spectrum, leading to a total integration time of approximately 15 min.

The Zugspitze CO columns are retrieved by integrating of profile retrievals which are performed by a simultaneous spectral fit in 3 micro-windows, i.e., 2057.7850–2057.9100 cm^{-1}, 2069.6150–2069.7100 cm^{-1}, and 2157.3300–2159.1500 cm^{-1}. Note that the spectral boundaries of these micro-windows have been slightly modified as compared to previous publications (Pougatchev and Rinsland, 1995; Rinsland et al., 2000), in order to minimize systematic spectral residuals. We are using the optimal-estimation method as implemented in the SFIT2-retrieval software provided by NASA, and established in collaboration with NIWA (Pougatchev et al., 1995). The HITRAN-2000 molecular line parameters compilation was used (Rothmann et al., 2003), and daily p-T-profiles from the Munich radiosonde station (located 80 km to the north of the Zugspitze) have been utilized. For a-priori information, a CO vertical volume mixing ratio profile obtained from the MOPITT team (L. N. Yurganov, personal communication, 2002) was adopted. The covariances for the CO mixing ratio profile vectors were assumed to be diagonal with the assumed uncertainties increasing by a factor of 2 below 30 km relative to their values above this altitude. Absolute uncertainties were then tuned empirically to optimize the trade off between gaining information content and avoiding oscillating retrievals. The accuracies/precisions for total vertical column CO retrievals via integrated vertical profile retrievals from ground-based FTIR measurements are understood and well characterized (Pougatchev and Rinsland, 1995; Rinsland et al., 2000). The actual numbers depend somewhat on changing geophysical parameters like the actual solar zenith angle. The random errors for single column retrievals have been estimated to be within ±2.5% and systematic errors to range from ±2.5 to ±5% (Pougatchev and Rinsland, 1995; Rinsland et al., 2000).

3. Validation approach

The retrieval of WFMD ver. 0.4 total column products of CO includes an empirical column scaling factor, i.e., WFMD CO data have been scaled to match MOPITT columns and a final scaling factor of 0.5 has been fixed for current and near future retrievals (Buchwitz et al., 2004). It is no near-future priority of the Bremen Science team to improve/update this scaling factor. Therefore, validation of absolute column values on overall average is not of interest. Rather, validation focus is put in our study on relative accuracy, i.e., investigating whether the atmospheric variabilities above the Zugspitze, which are dominated by the annual cycle for these species, can be retrieved from the SCIAMACHY data.

Individual WFMD retrievals in the near-infrared spectral domain are showing a significant scatter. This is because the small spectral signals are only slightly above the noise level, and because of the occurrence of systematic spectral residuals which are not understood yet (Buchwitz et al., 2004). Therefore, our validation approach is investigating to what extent the quality of SCIAMACHY data allows to reproduce the true variability of CO columns which is mainly dominated by the annual cycle above the Zugspitze, in a statistically significant manner. For this purpose, the annual cycle found by the Zugspitze FTIR column measurements is compared to the available time series of SCIAMACHY WFMD columns (data for ≈30 days in the time span January–October 2003) using daily mean pixel averages within a stepwise increased selection radius around the Zugspitze ground site. The goal is to thereby stepwise reduce the scatter of the daily means by statistically averaging over increasing ensembles of pixels.

One might argue that also polluted regions may be more and more included into the ensemble while increasing the selection radius, and this could potentially be compensating the statistical effect of reducing the scatter of the daily means. However, this effect is obviously weaker than the reduction of scatter by the statistical effect of increasing the averaging ensemble, as our test in Section 4 below is proving (Table 1). Furthermore, we are investigating in this study whether the CO annual cycle can be retrieved, and in our recent study on total column and in situ series of CO (Yurganov et al., 2004), it has been found, that the annual cycles of CO observed at a variety of stations within the northern hemisphere, are comparable at all stations as to phase and amplitude (≈10% amplitude, slightly lower for stations located within the free troposphere). This means, that increasing the selection radius for calculating daily means does not disturb the goal of obtaining a well defined annual cycle, but helps to reduce the scatter (see above).

Another issue of the validation approach is how to reduce the impact of varying ground altitudes of the different satellite pixels that are averaged on one hand, and, the different altitude of the Zugspitze mountain site on the other hand. We solve this problem in a 3-steps approach: i) All individual SCIAMACHY WFMD column values are normalized to coincident dry air column values which are also available from WFMD retrievals (via O_2 column retrievals). The resulting quantity is the so-called “dry air column averaged mixing ratio”. This quantity does not depend on the average pixel ground level altitude, assuming a constant mixing ratio with altitude. ii) To make the dry air column averaged mixing ratios of SCIAMACHY (unit ppbv) comparable to the FTIR column abundances above the Zugspitze (unit 1/cm^2), both data sets are then normalized to their overall average, and these (dimensionless) “anomalies” are used for validation/intercomparison purposes. iii) Finally, all individual Zugspitze columns

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are normalized to the daily mean local pressure. This is for consistency reasons, in order to make the Zugspitze ground data also independent from the actual pressure level, as the SCIAMACHY data are due to their normalization to the dry air column, see point i).

Finally, an important issue in intercomparing two different remote sounding systems (satellite versus ground) is to properly take their altitude dependent sensitivities, i.e., their averaging kernels (Rodgers, 1990) into account. In case of strongly differing kernels, neglecting the effect of different smoothing errors can result in intercomparison-errors in the order of the natural variability of the trace gas columns. However, in our case we encounter the nearly ideal situation, that the ground-based (FTIR) and satellite (SCIAMACHY) instruments are both sampling the CO columns with nearly the same total column averaging kernels as shown in Fig. 1, i.e., both being close to the ideal uniform sampling. There are only minor differences at higher altitudes, e.g., at the 300 hPa level, there is a slight under-estimation of the natural variability of ≈10% by FTIR, and a slight overestimation of ≈10% by SCIAMACHY. This means that we can directly compare the retrieved columns (satellite versus ground), and the intercomparison is not impacted significantly by (differing) smoothing errors. It is noteworthy, that the SCIAMACHY retrievals are perfectly sensitive down to the lower troposphere (as the ground-based measurements are, see Fig. 1). This is due to the near-infrared spectral domain utilized for the SCIAMACHY retrievals, and is advantageous over thermal-IR satellite retrievals which are showing a reduced sensitivity in the boundary layer.

4. Validation results

Figure 2 shows the available SCIAMACHY WFMD CO/O_2 column anomaly data (covering 33 days in 2003); each SCIAMACHY point is the average of all pixels from one day within a 2000-km radius around the Zugspitze, with the cloud flagged pixels removed. Note, that we did not restrict WFMD data selection to any maximum threshold in the individual retrieval errors reported, since we did not find any significant reduction of the scatter of daily means by testing such a restriction (errors below 100%). Four obvious outliers in the SCIAMACHY data have ad hoc been removed for Fig. 2 (the retrieval error for the strongest outlier is 20%). Zugspitze FTIR daily mean column anomalies are shown in the same plot. A 3rd order polynomial fit to the FTIR data nicely shows the CO annual cycle with a ≈10% amplitude.

To investigate whether information on this annual cycle can also be retrieved from SCIAMACHY data in a statistically significant manner, a linear fit to both SCIAMACHY and FTIR data is performed, see Fig. 3. It can bee seen from Fig. 3, that the slope of the linear fits of both data sets agree quite well. Table 1 shows the errors for the slopes of these linear fits for both FTIR and SCIAMACHY data sets, which were calculated using conservative error approximations for the daily means. It can be seen, that also for SCIAMACHY data the error of the slope is significantly smaller than the value of the slope itself and the regression coefficient is reasonably good ($R=-0.7$). This means that the obtained negative slope, which is due to the annual cycle, can be retrieved in a statistically significant manner, from SCIAMACHY WFMD data, given the considered selection radius of SCIAMACHY pixels of 2000 km around the Zugspitze.

The question to be addressed now is, what the minimum selection radius is, in order to obtain the negative slope in a statistically significant manner. Table 1 shows the regression results for a reduced selection radius of 1000 km. Now, the error of the slope is comparable to the absolute value of the slope. I.e., the negative slope, being a signature of the CO annual cycle, can no longer be retrieved in a statistically significant manner from the SCIAMACHY data. So our finding is, that a minimum selection radius of 1000–2000 km around Zugspitze is necessary, in order to retrieve the negative slope due to the CO annual cycle in a statistically significant manner from WFMD SCIAMACHY data.

Finally, we investigate, whether the information content in the SCIAMACHY data as to the annual cycle could be increased by including cloud flagged pixels also into the daily average. This question arises, since the cloud clearing algorithm applied is rather conservative (Buchwitz et al., 2004). Table 1 shows the result for the case of a 1000-km selection radius. In fact, including cloud flagged pixels does essentially not change the fit quality (slope error and R). This confirms that the cloud clearing algorithm is rather conservative.

5. Conclusions

Solar FTIR measurements at the Permanent Ground-Truthing Station Zugspitze (47.42° N, 10.98° E, 2964 m a.s.l.), Germany were used to validate the ENVISAT/SCIAMACHY Scientific Data Product for total column CO retrieved at the University of Bremen, i.e., the near infrared WFM-DOAS ver. 0.4 product.

The CO total column averaging kernels of the ground-based FTIR technique (integrated profile retrievals) turned out to be nearly identical to the SCIAMACHY WFMD kernels, which both maintain a nearly uniform sampling down to the lower troposphere with only minor differences at higher altitudes. Therefore a direct comparison of columns is possible without introducing significant intercomparison errors from differing smoothing errors.

In order to reduce the impact of varying ground altitudes of the different satellite pixels used for intercomparison, a new approach has successfully been explored. I.e., SCIAMACHY WFMD columns have been normalized to dry air columns, which have additionally been normalized to their overall average, and these anomalies then been compared to the ground FTIR column anomalies, to make both satellite and ground data sets comparable.

The infrared WFMD column retrievals include an empirical scaling factor of 0.5 which resulted from an adaptation to MOPITT data, therefore it is no issue to validate their overall absolute accuracy. Rather, focus was put on validating relative accuracy, i.e., investigating to what extent the quality of SCIAMACHY data (precision limited by spectral noise and systematic spectral residuals) allows to reproduce the actual variability of the CO columns, which is mainly dominated by the annual cycle, in a statistically significant manner. For this purpose, the annual cycle found by the Zugspitze FTIR

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column measurements (≈10% amplitude) was compared to the available time series of SCIAMACHY WFMD columns (i.e., January–October 2003) using daily mean pixel averages calculated from a stepwise increased selection radius around the Zugspitze. The resulting trade off was investigated between reducing the scatter in SCIAMACHY data by improving the statistics and introducing additional variabilities from emission sources. It was demonstrated that an increasing selection radius helps in reducing the scatter of CO. As a result it was found that, in order to obtain a statistically significant linear fit to the CO annual cycle (≈10% amplitude) from SCIA WFMD data, all pixels within a radius of at least 1000–2000 km around Zugspitze had to be averaged for each day.

In an upcoming study, when a final (maximum) set of CO columns will have been retrieved from all exploitable SCIAMACHY measurements of one year, it will be interesting to further investigate, whether also higher order momenta of the inter-annual variability (sinusoidal cycle, column anomalies) can be retrieved from SCIAMACHY data.

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Table 1. Slope, slope error, and regression coefficient R from the linear fit to the "Zugspitze FTIR" data, and to the SCIAMACHY CO data for a 2000-km pixel-selection radius around the Zugspitze ("SCIA 2000") as shown in Fig. 3. "SCIA 1000" means a 1000-km selection radius, and "SCIA 1000_cl" is with cloud flagged pixels included.

	Slope	Slope error	R
Zugspitze FTIR	−9.5E-4	±9.8E-5	−0.70
SCIA 2000	−1.2E-3	±4.9E-4	−0.43
SCIA 1000	−6.4E-4	±5.9E-4	−0.21
SCIA_cl 1000	−4.4E-4	±4.3E-4	−0.18

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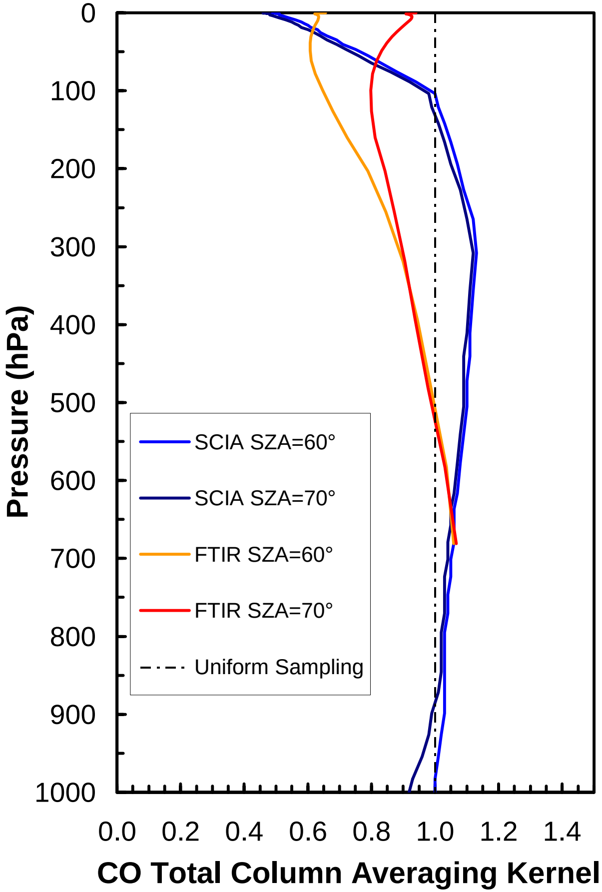

Fig. 1. Total column averaging kernels for Zugspitze FTIR and SCIAMACHY CO retrievals calculated for solar zenith angles of 60° and 70°.

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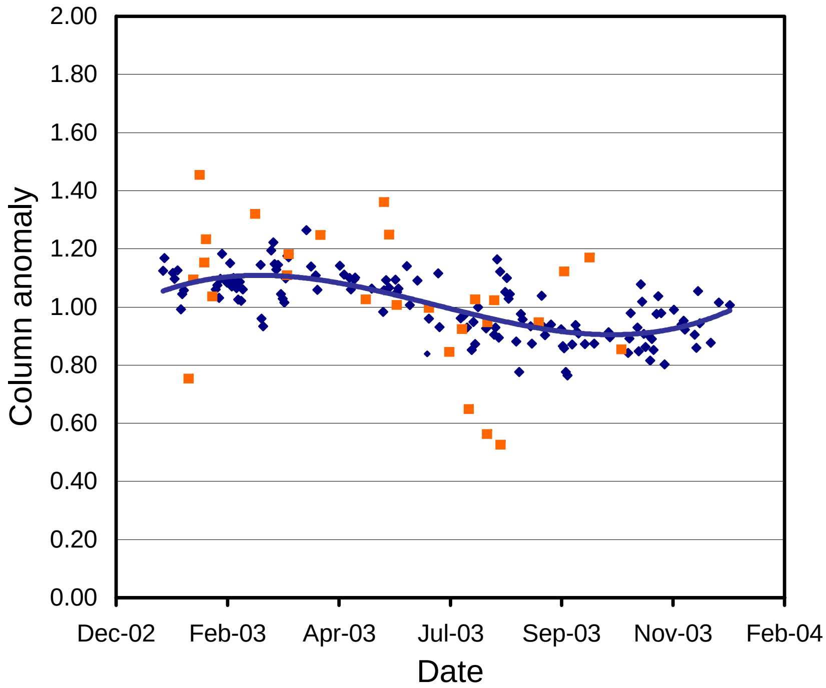

Fig. 2. Orange points: SCIAMACHY WFMD v0.4 CO/O_2 column anomaly: average of all pixels within a 2000-km radius around Zugspitze for daily overpass; cloud flagged pixels and 4 outliers removed. Blue points: Zugspitze FTIR CO column anomaly: daily means of pressure corrected columns. Blue line: 3rd order polynomial fit to the Zugspitze FTIR data.

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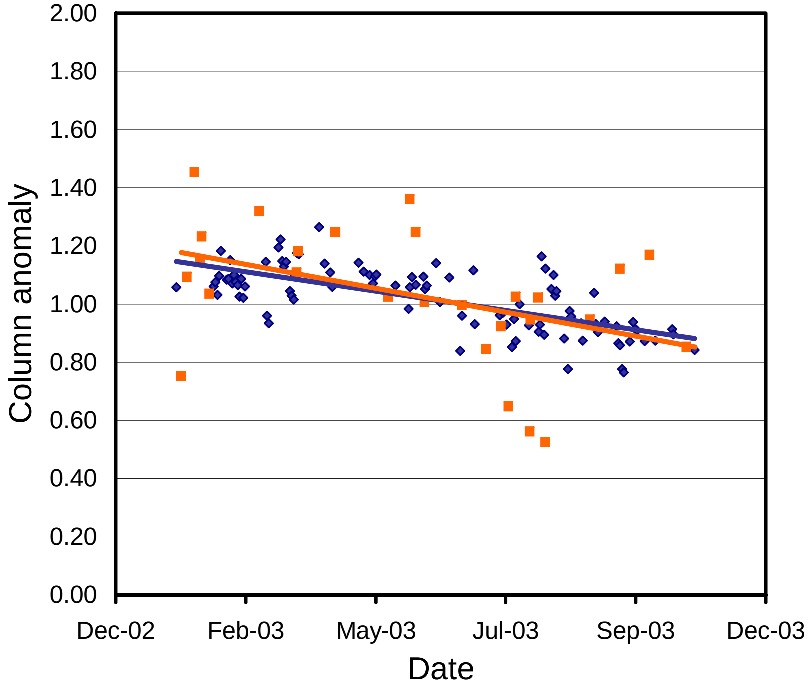

Fig. 3. Same CO data as Fig. 2, but the plotted time span of Zugspitze FTIR data is reduced to match the time span of available SCIAMACHY WFMD data. Solid lines: Linear fits. See Table 1 for the fit parameters.

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